

Single-file Diffusion with Random Diffusion Constants

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The single-file problem of N particles in one spatial dimension is analyzed, when each particle has a randomly distributed diffusion constant D sampled in a density $\rho(D)$. The averaged one-particle distributions of the edge particles and the asymptotic ($N \gg 1$) behaviours of their transport coefficients (anomalous velocity and diffusion constant) are strongly dependent on the D -distribution law, broad or narrow. When ρ is exponential, it is shown that the average one-particle front for the edge particles does not shrink when N becomes very large, as contrasted to the pure (non-disordered) case. In addition, when ρ is a broad law, the same occurs for the averaged front, which can even have infinite mean and variance. On the other hand, it is shown that the central particle, dynamically trapped by all others as it is, follows a narrow distribution, which is a Gaussian (with a diffusion constant scaling as N^{-1}) when the fractional moment $\langle D^{-1/2} \rangle$ exists and is finite; otherwise ($\rho(D) \propto D^{\alpha-1}$, $\alpha \leq \frac{1}{2}$), this density is, far from the origin, a stretched exponential with an exponent in the range $]0, 2]$; then the effective diffusion constant scales as $N^{-\beta}$, with $\beta = 1/(2\alpha)$.

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I. INTRODUCTION

The single-file diffusion problem is encountered in various fields (one-dimensional hopping conductivity [1], ion transport in biological membranes [2,3], channelling in zeolites [4]). Generally speaking, this is modelled by a set of N diffusing particles on the line with hard-core repulsion; due to such an interaction, any initial ordering is preserved in the course of time and the particles can be, once for all, labelled $1, 2, \dots, N$ from left to right. As in ref [5], I will here consider the case where, at the initial time, these particles form a compact cluster centered at the origin; the solution for an arbitrary initial condition has been given in ref [6], using the reflection principle. In addition, as contrasted to the standard model in which all the particles have the same diffusion constant D , it is here assumed that the particle i has a random D_i , chosen independently of all the others in a given distribution law $\rho(D)$. The latter can always be written as follows:

$$\rho(D) = \frac{1}{D_0} r\left(\frac{D}{D_0}\right), \quad (1.1)$$

where D_0 denotes a specific value of the diffusion constant (*e. g.* the average value) and $r(\xi)$ a positive function normalized to unity:

$$\int_0^{+\infty} r(\xi) d\xi = 1, \quad (1.2)$$

On a physical level, a random diffusion constant D can arise in various ways. For instance, by Stokes law and Einstein relation, it can result from a random radius; more directly, this also happens for particles having random masses.

The main purpose of this paper is to analyze how the choice of the distribution r modifies the large- N dependence of the transport coefficients for one particle of the cluster and, more generally, to find out the density probability of its coordinate in the presence of random diffusion constants. More specifically, focus will be given on edge particles and on the one which (for N odd) is at the middle of the cluster; for the “pure” case (all the particles have the same D), asymptotic laws ($N \gg 1$) have been given in ref. [5]. Among other results, it was shown that increasing N yields a narrowing of the one particle-probability distributions, as a result of the “pressure” exerted by other particles on a

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given one. This will be shown not to be true in all cases when the D 's are randomly sampled. As a rule, if the middle particle is most often insensitive to disorder – provided that the average $\langle D^{-1/2} \rangle$ exists and is finite – it will be shown that the distribution for the side particles strongly depends on the latter, going from narrow to broad laws.

II. BASIC RELATIONS

The diffusion equation here writes:

$$\frac{\partial}{\partial t} p(x_1, x_2, \dots, x_N; t) = \sum_{n=1}^N D_n \frac{\partial^2}{\partial x_n^2} p(x_1, x_2, \dots, x_N; t) . \quad (2.1)$$

As a consequence of the hard-core repulsion and of the above-mentioned initial condition, the solution has the expression:

$$p(x_1, x_2, \dots, x_N; t) = C_N \prod_{n=1}^N \frac{e^{-x_n^2/(4D_n t)}}{\sqrt{4\pi D_n t}} \prod_{n=1}^{N-1} Y(x_{n+1} - x_n) \quad (2.2)$$

In (2.2), Y is the Heaviside unit step function ($Y(x) = 1$ if $x > 0$, 0 otherwise), D_n denotes the diffusion constant of the n^{th} particle and C_N is the normalization constant. Since the D 's are assumed to be statistically independent, the various averages can be readily performed and the average N -particle front turns out to be:

$$\langle p(x_1, x_2, \dots, x_N; t) \rangle = N! \prod_{n=1}^N \langle G(x_n, t) \rangle \prod_{n=1}^{N-1} Y(x_{n+1} - x_n) , \quad (2.3)$$

where $\langle G(x_n, t) \rangle$ is the average of the gaussian distribution with the density $\rho(D)$:

$$\langle G(x_n, t) \rangle = \int_0^{+\infty} dD \rho(D) \frac{e^{-x_n^2/(4Dt)}}{\sqrt{4\pi Dt}} \equiv \frac{1}{(4D_0 t)^{1/2}} f(u_n) \quad (2.4)$$

where:

$$f(u) = \frac{1}{\pi^{1/2}} \int_0^{+\infty} d\xi \xi^{-1/2} r(\xi) e^{-u^2/\xi} \quad u_n = \frac{x_n}{(4D_0 t)^{1/2}} . \quad (2.5)$$

f is an even positive function normalized to $\frac{1}{2}$ on the interval $[0, +\infty]$.

From (2.3), all the one-particle averaged fronts can be formally obtained by integrating over all x 's but one:

$$\langle p_n^{(1)}(x_n; t) \rangle = \left(\prod_{m=1, m \neq n}^N \int_{-\infty}^{+\infty} dx_m \right) \langle p(x_1, x_2, \dots, x_N; t) \rangle . \quad (2.6)$$

One then finds:

$$\langle p_n^{(1)}(x; t) \rangle = \frac{N!}{(n-1)!(N-n)!} \left[\frac{1+I(u)}{2} \right]^{n-1} \left[\frac{1-I(u)}{2} \right]^{N-n} \frac{1}{(4D_0 t)^{1/2}} f(u) , \quad (2.7)$$

where $I(u)$ is defined by:

$$I(u) = 2 \int_0^u du' f(u') = \int_0^{+\infty} d\xi r(\xi) \Phi(u/\sqrt{\xi}) \equiv \langle \Phi(u/\sqrt{\xi}) \rangle \quad (2.8)$$

where Φ denotes the probability integral [7]. In (2.7), the two factors $[1 \pm I(u)]/2$ represent the steric effects on the n^{th} particle due to all other ones. $I(u)$ is a non-decreasing odd function such that $I(\pm\infty) = \pm 1$ (for the pure case, one simply has $I(u) = \Phi(u)$). For the edge particles ($n = 1$ or $n = N$), $\langle p_n^{(1)}(x; t) \rangle$ can be given a form occurring also in the theory of extreme events [8], namely:

$$\langle p_{1,N}^{(1)}(x;t) \rangle = \pm \frac{1}{(4D_0t)^{1/2}} \frac{d}{du} P_{\pm}(u) \quad P_{\pm}(u) = \left[\frac{1 \pm I(u)}{2} \right]^N . \quad (2.9)$$

The $-$ sign (resp $+$) refers to the left particle ($n = 1$) (resp. right particle ($n = N$)). In any case, the following relation holds true:

$$\langle p_1^{(1)}(x;t) \rangle = \langle p_N^{(1)}(-x;t) \rangle . \quad (2.10)$$

For n arbitrary, (2.9) generalizes into:

$$\langle p_n^{(1)}(x;t) \rangle = \frac{1}{(4D_0t)^{1/2}} C_N^n \left[\frac{d}{du} \left(\frac{1+I(u)}{2} \right)^n \right] \left(\frac{1-I(u)}{2} \right)^{N-n} . \quad (2.11)$$

For the particle which is at the center of the cluster (N odd), one has:

$$\langle p_{(N+1)/2}^{(1)}(x;t) \rangle = \frac{1}{(4D_0t)^{1/2}} \frac{N!}{\{[(N-1)/2]!\}^2} \left[\frac{1-I^2(u)}{4} \right]^{(N-1)/2} f(u) , \quad (2.12)$$

or, equivalently, from (2.11):

$$\langle p_{(N+1)/2}^{(1)}(x;t) \rangle = \frac{1}{(4D_0t)^{1/2}} C_N^{(N+1)/2} \left[\frac{d}{du} \left(\frac{1+I(u)}{2} \right)^{(N+1)/2} \right] \left(\frac{1-I(u)}{2} \right)^{(N-1)/2} . \quad (2.13)$$

In the following sections, the above equations will be used with different choices for the distribution $r(\xi)$. Exact asymptotic results for large N can be obtained due to the fact that, for $N \gg 1$, the steric factors $\{\frac{1}{2}[1 \pm I(u)]\}^n$ display a rather sharp variation.

Generally speaking, the one-particle transport coefficients can be found from the behaviour at small k of the characteristic function $\Pi_n(K)$:

$$\Pi_n(K) = \int_{-\infty}^{+\infty} dx e^{ikx} \langle p_n^{(1)}(x;t) \rangle \quad (K = k\sqrt{4D_0t}) . \quad (2.14)$$

The transport properties of the n^{th} particle subjected to the random field of all the other are essentially described by the two first cumulants:

$$\langle x_n \rangle(t) = V_{1/2,n}(N) \sqrt{t} \quad \Delta x_n^2 \equiv \langle x_n^2 \rangle(t) - [\langle x_n \rangle(t)]^2 = 2D_n(N)t . \quad (2.15)$$

The above time-dependences come from the fact that the only available length-scale is $(D_0t)^{1/2}$, so that $\langle x^\lambda \rangle \propto t^{\lambda/2}$ at all times and for any λ . Thus, at any time, the drift is always anomalous (no velocity) and the mean square displacement always has a purely diffusive motion. The following relations are trivially verified:

$$\langle x_1 \rangle(t) = - \langle x_N \rangle(t) \quad \Delta x_1^2(t) = \Delta x_N^2(t) . \quad (2.16)$$

In addition to the one-particle transport coefficients, statistical correlations between the particles can be analyzed. For definiteness, focus will be given on the correlations between the two edge particles, altogether contained in the two-body density:

$$\langle p_{1,N}^{(2)}(x_1, x_N) \rangle = \left(\prod_{m=2}^{N-1} \int_{-\infty}^{+\infty} dx_m \right) \langle p(x_1, x_2, \dots, x_N; t) \rangle . \quad (2.17)$$

Using (2.3) – (2.5), one finds:

$$\langle p_{1,N}^{(2)}(x_1, x_N; t) \rangle = \frac{1}{4D_0t} N(N-1) \left[\frac{I(u_N) - I(u_1)}{2} \right]^{N-2} f(u_1) f(u_N) Y(u_N - u_1) . \quad (2.18)$$

III. EXPONENTIAL DISTRIBUTION

As a first simple example, let us choose:

$$\rho(D) = \frac{1}{D_0} e^{-D/D_0} . \quad (3.1)$$

Here, D_0 is the expectation value of D . From (2.5) and (2.8), one readily obtains:

$$f(u) = e^{-2|u|} \quad I(u) = \operatorname{sgn} u (1 - e^{-2|u|}) . \quad (3.2)$$

The reduced densities for the edge particles density can now be explicitly calculated from (2.9) with:

$$P_-(u) = \begin{cases} 2^{-N} e^{-2Nu} & \text{if } u \geq 0 \\ (1 - \frac{1}{2} e^{-2|u|})^N & \text{if } u \leq 0 \end{cases} \quad (3.3)$$

and $P_+(u) = P_-(-u)$. From (3.3), the generating functions $\Pi_{1,N}(K)$ (2.14) for the edge particles are found as the following:

$$\Pi_1(K) = 1 + iK \left[\frac{1}{2^N(N - iK)} + \sum_{p=1}^N C_N^p \frac{(-1)^p}{p + iK} \right] \quad \Pi_N(K) = \Pi_1^*(K) . \quad (3.4)$$

Now, by expanding $\Pi_{1,N}$ in the vicinity of $K = 0$, and by coming back to the x -variable, one obtains:

$$\langle x_N \rangle(t) = - \langle x_1 \rangle(t) = [\ln(N/2) + C + O(2^{-N})] \sqrt{D_0 t} \equiv V_{1/2, \text{edge}}(N) \sqrt{D_0 t} \quad (3.5)$$

where C is the Euler's constant ($C = 0.577 \dots$). The mean square displacements are:

$$\Delta x_N^2 = \Delta x_1^2 = \left[\frac{\pi^2}{6} + O(2^{-N}) \right] D_0 t \equiv 2D_{\text{edge}}(N) t . \quad (3.6)$$

As compared to the pure case, the large- N behaviour of the transport coefficients is frankly different. When all the particles have the same diffusion constant, one has [5]:

$$V_{1/2, \text{edge}}^{(\text{pure})}(N) \propto (\ln N)^{\frac{1}{2}} \quad D_{\text{edge}}^{(\text{pure})}(N) \propto (\ln N)^{-1} . \quad (3.7)$$

As contrasted, for exponentially distributed random D , the anomalous drift coefficient increases like $\ln N$, whereas the effective diffusion constant $D_{\text{edge}}(N)$ tends towards a *finite* (non-vanishing) value. Also note that the height of the maximum also saturates and does not go to zero for N infinite. As a whole, the effect of an exponential disorder is rather subtle: most particles of the cluster have a rather small D , so that the pressure they exert on the edge ones is smaller than in the pure case; on the other hand, large D forces the packet to move with a “velocity” which increases more rapidly with N than in the pure case. The interplay of these facts produces a distribution having a finite height and width at infinite N . This is illustrated on Fig. 1, which clearly shows the width and height saturation when N becomes very large, as quantitatively described in eq. (3.6). It is readily seen that the value of $\langle p_{1,N}^{(1)} \rangle$ at its maximum is close to $(2/e) \propto N^0$.

For $N \gg 1$, the abscissa of the edge particles are approximately distributed according to:

$$\langle p_N^{(1)}(x; t) \rangle \simeq Y(u) \frac{N}{(4D_0 t)^{1/2}} e^{-(N/2)e^{-2u}} e^{-2u} \quad \langle p_1^{(1)}(x; t) \rangle = \langle p_N^{(1)}(-x; t) \rangle . \quad (3.8)$$

These functions are exponentially small ($\sim e^{-N}$) near $|u| = 0$ and display a plain exponential decay ($\sim e^{-2|u|}$) for $|u| \gg \ln[(N/2)^{1/2}]$. $\langle p_N^{(1)} \rangle$ is maximum for $u = u_{\text{max}} = \frac{1}{2} \ln(N/2)$; this shows that the corresponding x_{max} coincides with $\pm \langle x_N \rangle$ (see (3.5)). The approximate expressions (3.8) are hardly distinguishable from their exact counterparts as soon as N is greater than a rather small number ($\simeq 50$) and can be rewritten in terms of the proper shifted (but here not rescaled) variable X :

$$\langle p_N^{(1)}(x; t) \rangle \simeq Y(x) \frac{1}{(D_0 t)^{1/2}} e^{-e^{-x}} e^{-x} \quad X = \frac{x - x_{\text{max}}}{(D_0 t)^{1/2}} \quad x_{\text{max}} = (D_0 t)^{1/2} \ln(N/2) . \quad (3.9)$$

The statistical correlations between the two edge particles are most simply measured by the correlator C_{1N} :

$$C_{1N} = \langle x_1 x_N \rangle - \langle x_1 \rangle \langle x_N \rangle \quad (3.10)$$

which, due to scaling in space, varies linearly in time. C_{1N} can be found by using (2.18) and (3.2); for $N \gg 1$, a little algebra yields:

$$C_{1N} = 4 D_0 t [\ln^2(N/2) + O(\ln N)] \quad (3.11)$$

By (3.6), this implies that the normalized ratio $C_{1N}/\Delta x_{1,N}^2$ – which is constant in time – has a logarithmic increase with N :

$$\frac{C_{1N}}{\Delta x_{1,N}^2} \simeq \frac{6}{\pi^2} \ln^2(N/2) \text{ labelcorrexpnorm} \quad (3.12)$$

Although the numerator and the denominator of the ratio have separately different behaviours as compared to the pure case, the ratio still has a $\sim (\ln N)^2$ increase with N , exactly as in this latter case [5].

For the particle located at the middle of the cluster, the expression (2.13) writes:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle = \frac{1}{(4D_0 t)^{1/2}} \frac{1}{2} C_N^{(N+1)/2} \left(1 - \frac{1}{2} e^{-2|u|} \right)^{(N-1)/2} e^{-(N+1)|u|} \quad (3.13)$$

From (3.13), the following large- N expression of the mean square dispersion is obtained:

$$\Delta x_{(N+1)/2}^2(x; t) = \frac{1}{2} D_0 t C_N^{(N+1)/2} \left[B\left(\frac{N+1}{2}, \frac{N+1}{2}\right) - 4B\left(\frac{N+3}{2}, \frac{N+3}{2}\right) \right] \quad (3.14)$$

where B denotes the Euler beta-function [7]. Expansion for large- N yields:

$$\Delta x_{(N+1)/2}^2(x; t) \simeq \frac{1}{N} D_0 t \quad (3.15)$$

and provides the asymptotic dependence of the diffusion constant:

$$D_{\text{middle}}(N) \simeq \frac{1}{2N} D_0 \quad (3.16)$$

This behaviour is the same as for the pure case [5]. Thus, for the exponential distribution, the transport coefficient of the central particle is essentially unaltered by disorder – as shown below this is also true for any r density having $\langle D^{-1/2} \rangle$ finite. The asymptotic density of the middle particle is obtained from (3.13) as the following:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq \left(\frac{N}{2\pi D_0 t} \right)^{1/2} e^{-2(|u| + N u^2)} \quad (3.17)$$

This function is normalized to unity up to N^{-1} terms. Apart from the cusp at $u = 0$ and outside the region $|u| \leq 1/N$, this is essentially a gaussian distribution, exactly as in the pure case. For large N , the cusp can even be ignored and the distribution looks like a Gaussian everywhere.

In fact, it can now be stated the conditions for the stochastic dynamics of the central particle to be unaffected by disorder; such a particle is stymied in some way due to other particles and it can be suspected that strong steric effects most often dominate, except perhaps when the distribution $\rho(D)$ gives a high probability to find very small D . The analysis goes as follows. For $N \gg 1$, it is readily seen that the distribution (2.12) assumes non-negligible values only for $|u| \ll 1$. This in turn allows to replace $I(u)$ by its small- u expansion; from (2.8) and (2.4), $f(0)$ exists and is finite provided that $\rho(D)$ is bounded by $D^{-\beta}$ ($\beta < \frac{1}{2}$) for $D \rightarrow 0$. This means that when ρ diverges at small D , this divergence is not too severe, which implies that finding a small D has not such a great probability. With this assumption, one has:

$$I(u) \simeq 2u f(0) \quad f(0) = \frac{1}{\pi} \int_0^{+\infty} d\xi \xi^{-1/2} r(\xi) \equiv \frac{1}{\pi} \left\langle \left(\frac{D_0}{D} \right)^{1/2} \right\rangle \quad (3.18)$$

Using Stirling formula, and expanding $e^{[(N-1)/2] \ln[1-4u^2 f^2(0)]}$, one eventually gets the asymptotic approximation:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq \left(\frac{N}{2\pi D_0 t} \right)^{1/2} f(0) e^{-2N f^2(0) u^2} . \quad (3.19)$$

Note that the approximation automatically generates a properly normalized density. So, for any $\rho(D)$ such that $\lim_{D \rightarrow 0} [D^{1/2} \rho(D)] = 0$, the middle particle is essentially distributed according a normal law, the width of which decreasing as $N^{-1/2}$, up to unessential numerical factors. The expression (3.19) can be written as a universal law in term of the proper scaled variable X :

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq \left(\frac{N}{\pi t} \right)^{1/2} \langle D^{-1/2} \rangle \frac{e^{-X^2/2}}{(2\pi)^{1/2}} \quad X = x \left(\frac{N}{\pi t} \right)^{1/2} \langle D^{-1/2} \rangle , \quad (3.20)$$

expressing as a whole the irrelevance of details about the D distributions for the central particle when $\rho(D)$ is bounded near $D = 0$ as stated above, which entails that the fractional moment $\langle D^{-1/2} \rangle$ exists and is finite. The opposite case is treated in the next section which deals with the Gamma-distribution.

IV. GAMMA DISTRIBUTION

As another example – which in fact contains the exponential distribution as a particular case – let us choose a Gamma distribution:

$$\rho(D) = \frac{1}{\Gamma(\alpha) D_0^\alpha} D^{\alpha-1} e^{-D/D_0} \quad (\alpha > 0) . \quad (4.1)$$

With (4.1), the expectation values of D and D^2 are respectively equal to αD_0 and $\alpha(\alpha+1)D_0^2$. The exponential distribution is recovered by setting $\alpha = 1$, whereas the pure case can be obtained by taking the limit $\alpha \rightarrow \infty$, $D_0 \rightarrow 0$, $\alpha D_0 = \text{const}$. The f function (2.5) is:

$$f(u) = \frac{2}{\sqrt{\pi} \Gamma(\alpha)} |u|^{\alpha-\frac{1}{2}} K_{\alpha-\frac{1}{2}}(2|u|) \quad (4.2)$$

where $K_{\alpha-\frac{1}{2}}$ is the Bessel function of imaginary argument [7]. $f(0)$ exists and is finite if $\alpha > \frac{1}{2}$:

$$f(0) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\alpha + \frac{1}{2})}{(\alpha - \frac{1}{2}) \Gamma(\alpha)} \quad (\alpha > \frac{1}{2}) \quad (4.3)$$

The large- N approximation of the one-particle densities can be obtained along the same lines as in the previous section, by using the approximate expression:

$$I(u) \simeq 1 - \frac{1}{\Gamma(\alpha)} |u|^{\alpha-1} e^{-2|u|} \quad (|u| \gg 1) . \quad (4.4)$$

Let us consider first the right particle; one has:

$$\langle p_N^{(1)}(x; t) \rangle \simeq Y(u) \frac{1}{(4D_0 t)^{1/2}} \frac{N}{\Gamma(\alpha)} e^{-\frac{N}{2\Gamma(\alpha)} u^{\alpha-1} e^{-2u}} u^{\alpha-1} e^{-2u} . \quad (4.5)$$

When $\alpha < 1$, *i. e.* when ρ diverges at small D , $\langle p_N^{(1)} \rangle$ is exponentially small near $x = 0$. On the contrary, for $\alpha > 1$, $\langle p_N^{(1)} \rangle$ strictly vanishes as $u^{\alpha-1}$, but this behaviour is realized on a very small interval, namely $u < N^{-1/(\alpha-1)}$, beyond which $\langle p_N^{(1)} \rangle$ remains exponentially small. On the other hand, at large u , $\langle p_N^{(1)} \rangle$ has essentially an exponential decay, so that all the average values $\langle x_N^m \rangle$ exist and are finite. $\langle p_N^{(1)} \rangle$ is maximum at u_{max} :

$$u_{\text{max}} \simeq \frac{1}{2} \ln \frac{N}{2\Gamma(\alpha)} . \quad (4.6)$$

Again, $x_{\text{max}} = (4D_0 t)^{1/2} u_{\text{max}}$ is the relevant rescaled variable, since (4.5) can be rewritten as follows:

$$\langle p_N^{(1)}(x; t) \rangle \simeq Y(u) \frac{1}{(D_0 t)^{1/2}} e^{-(u/u_{\text{max}})^{\alpha-1} e^{-2(u/u_{\text{max}})}} (u/u_{\text{max}})^{\alpha-1} e^{-2(u/u_{\text{max}})} . \quad (4.7)$$

This readily gives $\langle p_N^{(1)} \rangle_{\max} \propto N^0$ which in turns allows to guess that, as for the exponential case, one has $\langle x_N \rangle \propto \ln N$ and $\langle \Delta x_{1,N}^2 \rangle \propto N^0$; it thus turns out that detailed calculations for $\alpha \neq 1$ are indeed of little interest. Up to unessential numerical factors, the large- N asymptotic laws all belong to the same class for Gamma-distributed diffusion constants, the behaviours being rather easily obtained by considering the simpler exponential case $\alpha = 1$; the same obviously holds for statistical correlations between edge particles.

For the central particle, one has to distinguish the two cases $\alpha > \frac{1}{2}$ and $\alpha < \frac{1}{2}$. Due to (4.3), the first one is described by the general expression (3.20). On the contrary, for $\alpha < \frac{1}{2}$, one has:

$$f(u) \simeq \frac{2^{2\alpha-1}}{\Gamma(2\alpha) \cos \alpha\pi} |u|^{2\alpha-1} \quad (|u| \ll 1) . \quad (4.8)$$

This in turns entails that:

$$F(u) \simeq \frac{2^{2\alpha}}{\Gamma(2\alpha+1) \cos \alpha\pi} |u|^{2\alpha} \quad (|u| \ll 1) . \quad (4.9)$$

As a consequence, one obtains:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq \frac{\alpha A}{(D_0 t)^{1/2}} \sqrt{\frac{2N}{\pi}} e^{-(N/2) A^2 |u|^{4\alpha}} |u|^{2\alpha-1} \quad A = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\frac{1}{2} - \alpha)}{\alpha \Gamma(\alpha)} . \quad (4.10)$$

This shows that when the probability is very high to find quite small diffusion constants, the distribution for the central particle diverges at $x = 0$ (but is clearly integrable) and is essentially a stretched exponential when $|u|$ is large:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \propto \begin{cases} |u|^{-(1-2\alpha)} & \text{if } |u| \ll 1 \\ e^{-C|u|^{4\alpha}} & \text{if } |u| \gg 1 \end{cases} . \quad (4.11)$$

For $\alpha = \frac{1}{2}$, $f(u)$ is proportionnal to the Bessel function K_0 and the divergence is logarithmic. In this case, one has:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq -\frac{1}{(D_0 t)^{1/2}} \sqrt{\frac{2N}{\pi^3}} e^{-(16N/\pi^2) u^2 \ln|u|} \ln|u| \quad (4.12)$$

which entails:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \propto \begin{cases} -\ln|u| & \text{if } |u| \ll 1 \\ e^{-C'u^2} & \text{if } |u| \gg 1 \end{cases} \quad (\alpha = \frac{1}{2}) . \quad (4.13)$$

The divergence at $x = 0$ comes from the interplay of pressure and of the frequent occurrence of central particle with a very small D . From (4.10), one finds:

$$\Delta x_{(N+1)/2}^2 \simeq 8 \left[\frac{\Gamma(\alpha+1)}{\Gamma(\frac{1}{2}-\alpha)} \right]^{1/\alpha} \frac{\Gamma(\frac{1}{\alpha})}{\Gamma(\frac{1}{2\alpha})} \left(\frac{2N}{\pi} \right)^{-\frac{1}{2\alpha}} D_0 t . \quad (4.14)$$

Summing up, the effective diffusion constant for the central particle and for the Gamma distribution scales with N as follows:

$$D_{\text{middle}} \propto N^{-\beta} \quad (4.15)$$

with:

$$\beta = \begin{cases} 1 & \text{if } \alpha \geq 1/2 \\ \frac{1}{2\alpha} & \text{if } 0 < \alpha \leq 1/2 \end{cases} . \quad (4.16)$$

V. BROAD DISTRIBUTIONS

The two previously examples discard the interesting case in which the diffusion constants are sampled in a broad law, possibly devoid of usual first few moments (mean and variance). Obviously enough, such a case is interesting since the average front for the edge particles are expected to be strongly asymmetric and also quite diffuse, due to the pressure exerted by inner particles and the possibility of rather high diffusion constants. This fact even opens the possibility for the edge particles to be also distributed according a broad law, devoid of mean and variance. Generally speaking, I will now consider the case:

$$\rho(D) = \mu D_0^\mu Y(D - D_0) D^{-(\mu+1)} \iff r(\xi) = Y(\xi - 1) \xi^{-(\mu+1)} \quad (\mu > 0) . \quad (5.1)$$

All the moments $\langle D^k \rangle$ diverge for $k \geq \mu$.

With the distribution (5.1), the f function (2.4) can be expressed in terms of the incomplete γ function [7]:

$$f(u) = \frac{\mu}{\pi^{1/2}} u^{-(2\mu+1)} \gamma(\mu + \frac{1}{2}, u^2) . \quad (5.2)$$

Again, I am interested in the large- N limit, in which case the right particle density (2.9) assumes non-negligible values for u of the order of or greater than u_0 defined as:

$$\left[\frac{1 + I(u_0)}{2} \right]^N = \frac{1}{2} \iff u_0 \simeq \left[\frac{N}{\pi^{1/2} \ln 4} \Gamma(\mu + \frac{1}{2}) \right]^{1/(2\mu)} . \quad (5.3)$$

For genuine broad laws (μ small), u_0 is much greater than 1 even for moderately large values of N . This allows to state again that the large- u expansion of $I(u)$ is only relevant, and to substitute everywhere the approximate expression:

$$I(u) \simeq 1 - \frac{1}{\pi^{1/2}} \Gamma(\mu + \frac{1}{2}) u^{-2\mu} \quad (u \gg 1) . \quad (5.4)$$

Injecting this in (2.9) yields the large- N approximation, valid for $u > 0$:

$$\langle p_N^{(1)}(x; t) \rangle \simeq N \frac{\mu}{\pi^{1/2}} e^{-N \Gamma(\mu + \frac{1}{2}) / (2\pi^{1/2} u^{2\mu})} u^{-(2\mu+1)} \gamma(\mu + \frac{1}{2}, u^2) , \quad (5.5)$$

it being understood that $\langle p_N^{(1)} \rangle$ is exponentially small for $u < 0$ and can be considered as identically vanishing for $u < 0$; note that the expression (5.5) goes toward zero extremely rapidly when $u \rightarrow 0$, namely:

$$\langle p_N^{(1)} \rangle \sim e^{-\text{Cst } N/u^{2\mu}} . \quad (5.6)$$

On the other hand, this distribution is indeed a broad law in the wide sense, since (5.5) displays for any μ a power-law behaviour at (very) large u :

$$\langle p_N^{(1)}(x; t) \rangle \simeq N \frac{\mu}{\pi^{1/2}} \Gamma(\mu + \frac{1}{2}) u^{-(2\mu+1)} \quad (u \gg N^{1/(2\mu)}) . \quad (5.7)$$

Eqs. (5.6) and (5.7) show that the average front for the right particle is strongly asymmetric, displaying a rather steep increase on the left (towards the inner part of the cluster) and a very slow decrease on the other side, towards the free part of space. The result (5.7) entails that the moment $\langle u^m \rangle$ exists and is finite only if the following inequality is satisfied:

$$m < 2\mu . \quad (5.8)$$

Thus, for $\mu \leq \frac{1}{2}$, the expectation value of x (as well as all higher moments) is infinite. The one-particle distribution (plotted in Fig. 3 for a few values of N) can nevertheless be characterized by the value u_{\max} giving its maximum value, which turns out to coincide with u_0 (see (5.3)), except for numerical factors. It is readily verified that, accordingly, the value of $\langle p_{1,N}^{(1)} \rangle$ at its maximum is $\propto N^{-1/(2\mu)}$. As a whole, the maximum of $\langle p_N^{(1)}(x; t) \rangle$ moves in time as the following:

$$x_{\max}(t) \simeq 2 \left[\frac{N}{\pi^{1/2}} \Gamma(\mu + \frac{1}{2}) \frac{\mu}{2\mu + 1} \right]^{1/(2\mu)} (D_0 t)^{1/2} . \quad (5.9)$$

x_{\max} is here the relevant rescaled coordinate; agreement is quite good with the exact results (see Fig. 3).

Note that for $\mu \rightarrow \infty$, (5.7) shows that $\langle p_N^{(1)} \rangle$ decreases faster than any arbitrary power of u^2 , in agreement with [5]. Also note that no obvious measure of correlations here exists since for $\mu < 1$ the mean square dispersions are infinite.

VI. SUMMARY AND CONCLUSIONS

For the single-file diffusion problem with random diffusion constants, the asymptotic laws (large N) giving the transport coefficients and the averaged one-particle densities have been derived.

Generally speaking, the asymptotic distribution of the central particle is most often gaussian (see (3.19)), as a result of the fact that steric effects nearly always dominate; when this is the case, the dynamical trapping of this particle is insensitive to details describing the distribution $\rho(D)$ of the diffusion constants. On the other hand, when $\rho(D)$ diverges as $D^{-1/2}$ or faster at small D ($\rho(D) \propto D^{\alpha-1}$, $\alpha \leq \frac{1}{2}$), the distribution of the central particle is no more a normal one: at small x , it itself goes to infinity as $x^{-(1-2\alpha)}$ and is a stretched exponential $e^{-Cx^{4\alpha}}$ at large x (see (4.10)). The effective diffusion constant scales as $N^{-1/(2\alpha)}$ for $\alpha < \frac{1}{2}$ and as N^{-1} otherwise, showing that in the N -infinite limit, as in the pure case, the motion indeed becomes subdiffusive in agreement with Harris result [9].

On the contrary, the stochastic dynamics of the edge particles is strongly dependent upon the nature (narrow or broad) of the diffusion constants probability density $\rho(D)$. When the latter is narrow (*i. e.* exponential), the effective diffusion constant of edge particles tends toward a *finite* constant when N becomes infinite; the average coordinate increases with N as $\ln N$, faster than for the pure case. When the $\rho(D)$ is broad (*i. e.* behaves as a power law $D^{-(\mu+1)}$ at large D), the edge particles are themselves distributed according a broad law, devoid of mean and variance when μ is smaller than $\frac{1}{2}$. The distribution of the coordinate, strongly asymmetric (see Fig. 3), can nevertheless be characterized by the abscissa of its maximum (5.9); the prefactor of the latter displays a $N^{1/(2\mu)}$ scaling *i. e.* rapidly increases with N when μ is small. This comes from the fact that there is a high probability to find inner particles with a large diffusion constant which, in turns, gives rise to a high “pressure” exerted by the core of the cluster on its “surface”.

In all cases, the averaged one-particle asymptotic density has been found; it can be written under a general form displaying the basic ingredients of the problem. For the right particle, one has:

$$\langle p_N^{(1)}(x; t) \rangle \simeq N \exp \left[-\frac{N}{2} \langle 1 - \Phi[x/(4Dt)^{1/2}] \rangle \right] \langle G(x, t) \rangle . \quad (6.1)$$

where $\langle \dots \rangle$ denotes averaging with the distribution $\rho(D)$ of the diffusion constants, Φ is the probability integral and G is the gaussian distribution. For the central particle (N odd), one has:

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq \left(\frac{N}{2\pi^2 t} \right)^{1/2} \langle D^{-1/2} \rangle \exp \left[-N \langle D^{-1/2} \rangle \frac{x^2}{2\pi t} \right] , \quad (6.2)$$

provided that the fractional moment $\langle D^{-1/2} \rangle$ exists and is finite. Otherwise, when $\rho \propto D^{\alpha-1}$ at small D with $\alpha \leq \frac{1}{2}$, $\langle p_{(N+1)/2}^{(1)} \rangle$ is of the form (see (4.10) for details):

$$\langle p_{(N+1)/2}^{(1)}(x; t) \rangle \simeq C |x|^{-(1-2\alpha)} \exp [-C' |x|^{4\alpha}] . \quad (6.3)$$

At large x , this gives a stretched exponential with an exponent in the range $]0, 2]$, whereas the density diverges at $x = 0$ as a power-law ($\propto x^{-(2\alpha-1)}$); for the particular case $\alpha = \frac{1}{2}$, this singularity becomes logarithmic.

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Figure Captions

1. Exact averaged front $\langle p_1^{(1)}(x; t) \rangle$ for the left particle with exponentially distributed diffusion constants; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$. Each curve is labelled by the number of particles in the cluster.
2. Averaged front $\langle p_{(N+1)/2}^{(1)}(x; t) \rangle$ of the central particle (4.10) for a cluster of 10 particles when the diffusion constants are distributed according to (4.1) with $\alpha = \frac{1}{4}$; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$.
3. Exact averaged front $\langle p_N^{(1)}(x; t) \rangle$ for the right particle when the diffusion constants of the cluster are distributed according to (5.1) with $\mu = \frac{1}{2}$; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$. Each curve is labelled by the number of particles in the cluster.





